SMX 3161.2 (98-13DIV2)
PATENT

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Application of Shenheng Guan et al. Art Unit 1743
Serial No. 10/071,546
Filed February 8, 2002
Confirmation No. 9873
For APPARATUS FOR SCREENING CATALYSTS IN A PARALLEL FIXED-BED REACTOR
Examiner Dwayne K. Handy

DECLARATION OF PRIOR INVENTION UNDER 37 CFR § 1.131

I, Shenheng Guan, declare as follows:

1. I am currently an adjunct associate professor in the Department of Pharmaceutical Chemistry at the University of California, San Francisco.

2. From October, 1996 to January, 2002, I was employed as a Distinguished Scientist at Symyx Technologies, Inc. (Santa Clara, California), the assignee of the above-referenced U.S. patent application, Serial No. 10/071,546.

3. I am named as a joint inventor in the above-referenced patent application and I am the sole inventor of some of the claimed subject matter, including the invention defined in independent claims 61-63 and dependent claims 70 and 80-87 depending therefrom as currently amended and presented in Amendment C submitted herewith.

4. I conceived of and, with the assistance of other Symyx employees, reduced to practice in the United States the subject matter of the invention as defined in currently amended independent claims 61-63 and dependent claims 70 and 80-87 depending therefrom before February 19, 1998, the facts being set forth below.

5. The invention described and claimed in the subject patent application was developed as part of a materials research program that I participated in while employed at Symyx Technologies, Inc.

6. Exhibit A, attached to this Declaration, is a true and correct copy of an internal research report I prepared prior to February 19, 1998 in connection with the above-mentioned research program as part of my duties at Symyx Technologies, Inc. The report describes the conception and development of a parallel fixed-bed reactor for screening catalysts and evinces my conception of the subject matter of currently amended independent claims 61-63 and dependent claims 70 and 80-87 depending therefrom and reduction to practice of an operational "six-channel prototype reactor" prior to February 19, 1998.

7. All work referred to herein was carried out in the United States.

8. All statements that I made herein of my own knowledge are true and all statements made on information and belief are believed to be true. I acknowledge that willfully making false statements is punishable by fine, imprisonment, or both, under 18 U.S.C. § 1001 and that such willful false statements may jeopardize the validity of any patent issuing from this application.

Shenheng Guan

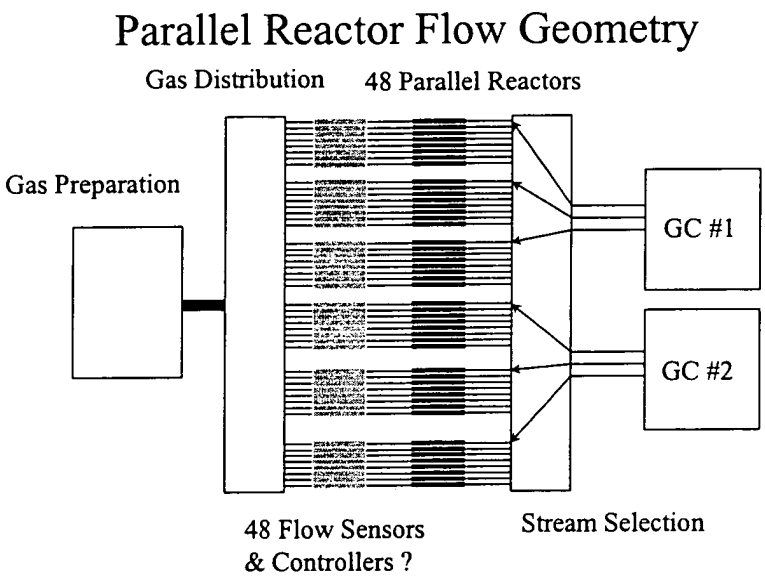
1/9/2006
Date

EXHIBIT A

Symyx Parallel Fixed Bed Reactor

Shenheng Guan

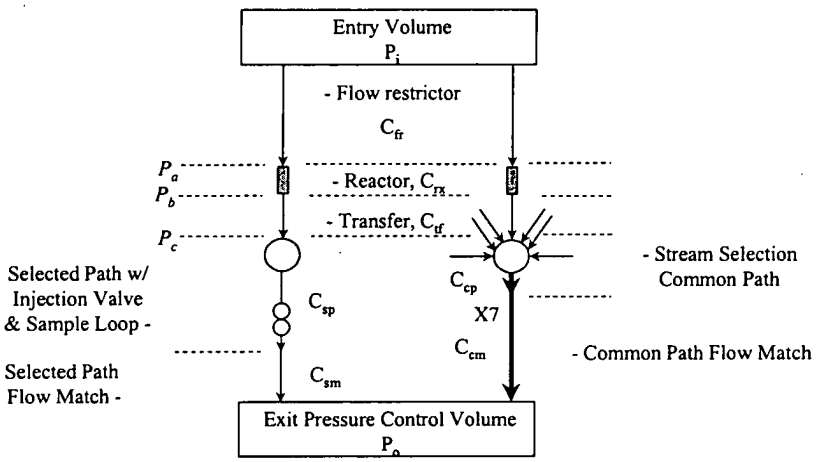
The Design philosophy of the parallel fixed bed reactor is to scale down from conventional laboratory reactors and to operate many reactors simultaneously. By choosing catalyst loading to be two orders of magnitude lower than that in conventional reactors, many catalysts can be synthesized quickly. Since many important parameters, such as space velocity, contact time, and power forms of catalyst, can be preserved, data from the reactor can often be compared with that from conventional methods directly. Final version of the parallel reactor contains 48 individual reactors.



Design of the parallel fixed bed reactor offers several advantages over single bed reactors. It allows creation of nearly identical reaction conditions for all the individual reactors and allows one to carry out catalyst activation and catalytic reactions simultaneously. With a careful design, reaction conditions for the individual reactors can be controlled – creating opportunities for combinatory studies of reaction conditions for the same catalyst. Six identical gas chromatography (GC) channels analyze products simultaneously. Since 48 reactors need to be analyzed, sophisticate gas distribution and stream selection valve control methods are introduced. By use of GC for detection, almost all possible reaction systems can be investigated. The parallelism of the reactor allows analysis process to be pipelined, therefore, characterization time can be minimized.

The key design concept of the reactor is to use flow restriction upstream from individual reactors. By supplying a common inlet pressure and a common outlet pressure, the flow rate of the individual reactor is determined mainly by conductance of the flow restriction.

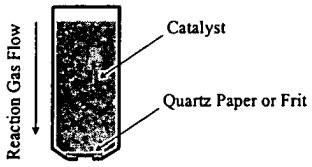
Parallel Reactor Flow Matching



If the flow restriction has conductance orders of magnitude smaller than that of the rest flow path and all reactors have the same flow restriction, the variation of conductance among reactors (for example, by catalyst packing) will not cause large variation in flow rate. Mass flow controllers premix reaction gas that is then supplied to all the reactors through a bundle of long and narrow bore capillaries (as flow restrictors). Flow measurement has been done on the six-channel prototype reactor. A flow variation of less than 2% was observed.

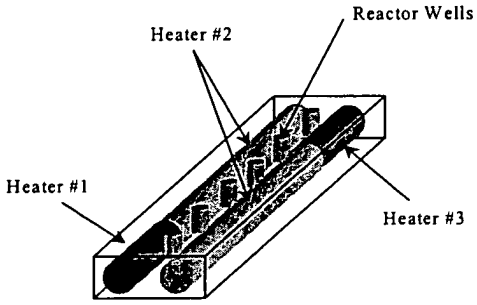
The prototype reactor block was constructed with stainless steel. Catalysts are contained in cartridges made of quartz or stainless steel.

Parallel Reactor Catalyst Cartridge



Quartz paper is used as frit to prevent power from escaping from the cartridge. The reaction block can be opened on the top to expose all the catalyst cartridges, allowing easy sample change. A three heating zone method is developed to achieve uniform temperature distribution among reactor wells.

Temperature Control Method in Parallel Reactor



The three zones are independently controlled with PID loops. A temperature spatial variation below 4°C at 350°C has been realized. The additional benefit from such method is a linear temperature gradient can be easily generated. A 10°C difference between adjacent reactors was obtained. Currently, the six-channel prototype reactor is operational and producing reliable data.